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We study the robustness of wavefunctions of interacting many bosons against the leakage of bosons, by deriving and analyzing a general equation of motion for the reduced density operator. We identify a robust wavefunction that remains a pure state, whereas other wavefunctions, such as the Bogoliubov's ground state and the ground state with a fixed number of bosons, evolve into mixed states. Although these states all have the off-diagonal long-range order, and the same energy, we argue that only the robust state is realized as a macroscopic quantum state.

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When a quantum system is subject to perturbations from its environment, most wavefunctions decohere, and only an exceptional wavefunction(s) remains pure. For quantum systems with a single degree of freedom ($f = 1$), this robust wavefunction is a coherent state [1,2]. For example, when a coherent state $|\alpha\rangle$ of single-mode photons passes through an absorptive medium, the final state is also a coherent state $|\alpha'\rangle$, which was attenuated ($|\alpha'| < |\alpha|$) by the absorption [1]. It was also argued from a master equation for a $f = 1$ system that coherent states produce the least entropy, thus being stable [2]. Since these conclusions are based on analyses on $f = 1$ systems, a natural question is: Are they applicable to macroscopic systems, i.e., to $f \gg 1$ interacting systems? Moreover, we must identify what coherent states are robust, because there are many choices of the coordinate by which a coherent state is defined. Furthermore, for massive bosons the superselection rule (SSR) forbids superpositions of states with different numbers of bosons. Hence, we must clarify how coherent states can be compatible with the SSR. The purpose of this *Letter* is to answer these questions for condensates of interacting many bosons, which (or, equivalents of which) are observed in many physical systems such as liquid He [3], quantum Hall systems [4], excitons [5], and trapped atoms [6]. We also discuss the symmetry breaking (SB) in view of the robustness.

We consider many bosons which interact each other repulsively. We assume that the bosons are confined in a large but finite box of volume V , which is placed in a huge room of volume $\mathcal{V} \gg V$, which we call the environment. Suppose that the potential of the walls of the box is not high enough, so that the box and the environment exchange bosons via tunneling processes at a small rate (flux) J . Let t_{eq} denote the time scale after which the total system, the box plus the environment, reaches the equilibrium state. We are not interested in the time region $t \geq t_{eq}$ because the equilibrium state is just a uniform state that is determined only by the initial state of the environment (because $\mathcal{V} \gg V$). We therefore examine the *transient region* for which $t \ll t_{eq}$, in order to discuss the robustness of an initial state $|\phi(0)\rangle$, which

is prepared at $t = 0$, of the box. Depending on the choice of the initial state $|\phi_E(0)\rangle_E$ of the environment, the box state may be affected either drastically or moderately. For example, a moderate situation is that $|\phi_E(0)\rangle_E$ has the same density n of bosons as $|\phi(0)\rangle$. In such a case, n of the box will be kept constant for all t . To discuss the robustness, however, we consider the severest situation where the environment is initially in the vacuum state $|0\rangle_E$ of bosons, so that bosons escape from the box continuously. If a box state is robust in this severest case, it would also be robust in other cases. Hence, the total wavefunction at $t = 0$ is $|\Phi(0)\rangle_{total} = |\phi(0)\rangle \otimes |0\rangle_E$. We decompose (the \mathbf{r} dependence of) the boson field that is defined on $V + \mathcal{V}$ as $\hat{\psi}_{total}(\mathbf{r}) = \hat{\psi}(\mathbf{r}) + \hat{\psi}_E(\mathbf{r})$. Here, $\hat{\psi}(\mathbf{r})$ localizes in the box, whereas the low-energy component of $\hat{\psi}_E(\mathbf{r})$ localizes in the environment [7]. Accordingly, the Hamiltonian of the total system is decomposed as $\hat{H}_{total} = \hat{H} + \hat{H}_E + \hat{H}_{SE}$. Here, \hat{H} (\hat{H}_E) is a function of $\hat{\psi}$ ($\hat{\psi}_E$) only, describing interacting bosons in the box (environment). On the other hand, \hat{H}_{SE} includes both $\hat{\psi}$ and $\hat{\psi}_E$, describing the $\hat{\psi}$ - $\hat{\psi}_E$ interaction. If the leakage flux J is small, the probability of finding two or more bosons simultaneously in the walls of the box is negligible, and thus the dominant term of \hat{H}_{SE} takes the following form:

$$\hat{H}_{SE} = \lambda \int d^3\mathbf{r} \hat{\psi}_E^\dagger(\mathbf{r}) w(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \text{H.c.} \quad (1)$$

Here, $w(\mathbf{r})$ represents the shapes of the walls ($w \sim 1$ in the walls, $w = 0$ in other regions), whose potential height is characterized by a parameter λ . Details of w are irrelevant because they are all absorbed in the value of j , Eq. (9). In the time region of interest ($t \ll t_{eq}$), the $\hat{\psi}_E$ - $\hat{\psi}_E$ interaction should be unimportant because n of the environment remains zero. On the other hand, we must treat the $\hat{\psi}$ - $\hat{\psi}$ interaction appropriately. For this purpose, we use the decomposition formula for $\hat{\psi}$ [8–10]:

$$\hat{\psi} = \hat{\Xi} + \hat{\psi}', \quad (2)$$

where $\hat{\Xi}$ is an operator introduced by Lifshitz and Pitaevskii (LP) [8]. We here define it slightly differently:

$$\hat{\Xi}|N, G\rangle = \sqrt{N}\xi|N-1, G\rangle, \quad (3)$$

where $|N, G\rangle$ denotes the ground state that has *exactly* N bosons [8,9,11], which we call the number state of interacting bosons (NSIB), and

$$\xi \equiv \langle N-1, G | \hat{\psi} | N, G \rangle / \sqrt{N} \quad (4)$$

is a hallmark of the condensation: $\sqrt{N}\xi = \mathcal{O}(1)$ for condensed states, whereas $\sqrt{N}\xi = \mathcal{O}(1/\sqrt{V})$ for normal states [8,9,12]. We here consider the condensed states. Since $\hat{\psi}$ alters N exactly by 1, Eq. (3) yields

$$\langle N - \Delta N, G | \hat{\psi} | N, G \rangle = \sqrt{N}\xi \delta_{\Delta N, 1}, \quad (5)$$

for all ΔN such that $|\Delta N| \ll N$. It then follows that $\langle N - \Delta N, G | \hat{\psi}' | N, G \rangle = 0$. Namely, $\hat{\psi}'$ transforms $|N, G\rangle$ into excited states.

For weakly-interacting bosons, the explicit forms of the NSIB were given in Refs. [9,11], and that of $\hat{\Xi}$ was given in [9]. Because of the boson-boson interaction, they are rather complicated functions of bare operators $\hat{a}_{\mathbf{k}}$: $|N, G\rangle = (1/\sqrt{N!})e^{i\hat{G}}(\hat{a}_0^\dagger)^N|0\rangle$ and $\hat{\Xi} = e^{i\varphi} \sqrt{n_0/nV} e^{i\hat{G}} \hat{a}_0 e^{-i\hat{G}}$. Here, $n_0 = \langle \hat{N} - \int d^3\mathbf{r} \hat{\psi}'^\dagger \hat{\psi}' \rangle / V$, $\hat{G} \equiv (-i/2nV) \hat{a}_0^\dagger \hat{a}_0^\dagger \sum_{\mathbf{q} \neq 0} y_{\mathbf{q}} \hat{a}_{\mathbf{q}} \hat{a}_{-\mathbf{q}} + \text{H.c.}$, φ is an arbitrary phase, and $y_{\mathbf{q}}$ is given in Ref. [9]. Using these expressions, we can show that [10]

$$[\hat{\Xi}, \hat{\Xi}^\dagger], [\hat{\Xi}, \hat{\psi}'], [\hat{\Xi}, \hat{\psi}'^\dagger] = \mathcal{O}(1/V). \quad (6)$$

LP claimed that Eq. (6) is applicable even when the interaction is stronger [8]. Their discussion is somewhat controversial because LP started from, instead of Eq. (3), the assumption that $\hat{\Xi}$ could be defined by $\hat{\Xi}|N, \nu\rangle = \Xi|N-1, \nu\rangle$, where $|N, \nu\rangle$ denotes *any* eigenstate that has exactly N bosons. However, we note that for weakly-interacting bosons we have not used this assumption in the derivation of Eq. (6). We thus expect that Eq. (6) also holds for bosons with stronger interaction, even if LP's assumption were too strong. If this is the case, the following results are applicable not only to weakly interacting bosons but also to bosons with stronger interaction, because the results will be derived only from Eqs. (1)-(6).

Since we are studying the robustness against *weak* perturbations, we assume that λ is small, so that J is very small. In this case, we have to consider transitions only among $|N, G\rangle$'s with different N 's (i.e., we can neglect transitions to excited states). Hence, the reduced density operator $\hat{\rho}$ can be generally written as

$$\hat{\rho}(t) = \sum_{N, M} \rho_{NM}(t) |N, G\rangle \langle M, G|. \quad (7)$$

It seems almost obvious that quantum coherence between $|N, G\rangle$ and $|M, G\rangle$ with large $|N-M|$ would be destroyed by the interaction with the environment. We therefore study the most interesting case where ρ_{NM} is localized in the N - M plane in such a way that $\sqrt{\langle \delta N^2 \rangle} \ll \langle N \rangle$.

If this relation is satisfied at $t=0$, it is also satisfied for all $t \ll t_{\text{eq}}$. We also assume that \mathcal{V} is large enough, so that the boson density in the environment ($= [\langle N(0) \rangle - \langle N(t) \rangle] / \mathcal{V}$) is negligibly small for all $t \ll t_{\text{eq}}$. Under these conditions, we can calculate the time evolution of $\rho_{NM}(t)$, using Eqs. (1)-(6), as [10,13]

$$\begin{aligned} \rho_{NM}(t + \Delta t) = & e^{-i(N-M)\mu(n(t))\Delta t/\hbar} \\ & \times [\rho_{NM}(t)(1 - (N+M)j(n(t))\Delta t/2) \\ & + \rho_{N+1, M+1}(t)\sqrt{(N+1)(M+1)}j(n(t))\Delta t] + \mathcal{O}(\lambda^4), \end{aligned} \quad (8)$$

for a finite time interval Δt that satisfies $\hbar/E_c \lesssim \Delta t < 1/\langle N \rangle j(n)$, where E_c is the energy scale over which the matrix elements of \hat{H}_{SE} are non-negligible. Here, $n \equiv \langle N \rangle / V$, and $\mu(n)$ (> 0 for a condensate of interacting bosons [3,8,9]) denotes the chemical potential of bosons in the box. Furthermore,

$$j(n) = K \frac{2\pi}{\hbar} \frac{n_0}{n} |\lambda|^2 \frac{v^2}{V} D(\mu(n)), \quad (9)$$

where $D(\mu)$ is the density of states per unit volume of the environment at energy μ , v is the total volume of the walls of the box, and K is a constant of order unity. Both μ and j depend on $\langle N \rangle$ through n , but this dependence is very weak because a change of $\langle N \rangle$ by 1 only causes the change of n by $1/V$. Note that Eq. (9) has only two parameters, μ and j . Namely, all model-dependent parameters (details of \hat{H} , \hat{H}_{E} and \hat{H}_{SE}) are absorbed in these two parameters. Therefore, the following results are general and model independent.

Using Eq. (8), we first calculate the time evolutions of the expectation value $\langle N \rangle$ and the fluctuation $\langle \delta N^2 \rangle$ of the number N of bosons in the box. We find

$$\frac{d}{dt} \langle N \rangle = -j(n) \langle N \rangle. \quad (10)$$

Hence, $\langle N \rangle$ decreases gradually because of the leakage flux $J = j(n) \langle N \rangle$. For $\langle \delta N^2 \rangle$, on the other hand, we find

$$\frac{d}{dt} F = j(n)[1 - F], \quad (11)$$

where $F \equiv \langle \delta N^2 \rangle / \langle N \rangle$ is the ‘‘Fano factor’’ [1]. It is found that a robust state must have $F = 1$, whereas any states with $F \neq 1$ are fragile in the sense that their F evolves with time, approaching unity. For example, the ground-state wavefunction in the Bogoliubov approximation, $|\text{Bog}, G\rangle$, has $F > 1$ [9]. Hence, it does *not* satisfy the robustness condition. Neither does the ground-state wavefunction with a fixed number of bosons, $|N, G\rangle$, because $F = 0$. Since the evaluation of F is easy, F is a convenient tool for the investigation of the robustness, as seen from these examples. However, since F is only related to the diagonal elements of $\hat{\rho}$, it does not distinguish between pure and mixed states. Therefore, to investigate

the robustness of wavefunction in more detail, we solve Eq. (8) for various initial states.

When the initial state is a pure state of the NSIB, i.e., $\hat{\rho}(0) = |N, G\rangle\langle N, G|$, then $\rho_{N'M'}$ after an short interval Δt is evaluated as $\rho_{NN}(\Delta t) = (1 - Nj(n(t))\Delta t)$, $\rho_{N-1, N-1}(\Delta t) = Nj(n(t))\Delta t$, and other elements are zero. Therefore, $\hat{\rho}$ becomes a classical mixture of $|N, G\rangle$ and $|N-1, G\rangle$ at $t = \Delta t$, in consistent with the above result that $F = 0$ is fragile. By evaluating the evolution at later times, we find that $\hat{\rho}$ evolves toward a Poissonian mixture of $|N, G\rangle$'s [13], in consistent with $F \rightarrow 1$.

In a similar manner, we can show that the pure state of Bogoliubov's ground state $\hat{\rho}(0) = |\text{Bog}, G\rangle\langle \text{Bog}, G|$, which has $F > 1$, also evolves into a mixed state. We can also show that the number-phase squeezed state of interacting bosons (NPB), which was found in Ref. [9] as a number-phase minimum uncertainty state with $0 < F < 1$, also evolves into a mixed state. These results show that F is indeed a simple measure of the robustness: A pure state with $F \neq 1$ is unlikely to remain pure. In other words, among states with $F = 1$ we may find a very special state that is robust in the sense that it remains pure when it is weakly perturbed by the environment. We now explore such a special state.

There are many wavefunctions which satisfy $F = 1$. For example, among such states is the coherent state of free bosons (CSFB), which we find evolves into a mixed state. Hence, $F = 1$ is only a necessary condition for the robustness. Among many states with $F = 1$, we have successfully found the robust state as

$$\hat{\rho}(t) = |\alpha(t), G\rangle\langle \alpha(t), G|. \quad (12)$$

Here, $\alpha(t)$ is a time-dependent complex number given by

$$\alpha(t) = e^{i\varphi(t)} \sqrt{\langle N(t) \rangle}, \quad (13)$$

where $\langle N(t) \rangle$ is the solution of Eq. (10), and

$$\varphi(t) = \varphi(0) - \frac{i}{\hbar} \int_0^t \mu(n(t)) dt. \quad (14)$$

Here, the initial phase $\varphi(0)$ is arbitrary, and $n(t) \equiv \langle N(t) \rangle / V$. Furthermore,

$$|\alpha, G\rangle \equiv e^{-|\alpha|^2/2} \sum_{M=0}^{\infty} \frac{\alpha^M}{\sqrt{M!}} |M, G\rangle, \quad (15)$$

which we call the coherent state of interacting bosons (CSIB). It has the same form as the CSFB except that $|M, G\rangle$ is the NSIB. Because of this difference, simple relations for the CSFB do not hold for the CSIB. For example, $\langle \alpha, G | \hat{\psi} | \alpha, G \rangle \neq \alpha / \sqrt{V}$, and, moreover, $|\alpha, G\rangle$ is not an eigenstate of $\hat{\psi}$. Nevertheless, $\langle \alpha, G | \hat{N} | \alpha, G \rangle = \langle \alpha, G | \delta \hat{N}^2 | \alpha, G \rangle = |\alpha|^2$, hence $F = 1$ exactly, as in the case of CSFB. Since the NSIB has a complicated wavefunction, so does the CSIB. [For weakly-interacting

bosons, its explicit form was given in Ref. [9].] Although complicated, the wavefunction of the CSIB is robust against the perturbations from the environment. It keeps the same form, whose parameter $\alpha(t)$ evolves slowly (except for the phase rotation), and remains a pure state, in contrast to other wavefunctions which soon evolve into mixed states. In fact, Eqs. (12)-(15) yield

$$\rho_{NM}(t) = e^{-\langle N(t) \rangle} \frac{e^{i(N-M)\varphi}}{\sqrt{N!M!}} \langle N(t) \rangle^{\frac{N+M}{2}}, \quad (16)$$

$$\begin{aligned} \rho_{NM}(t + \Delta t) &= e^{-\langle N(t) \rangle (1-j\Delta t)} \frac{e^{i(N-M)(\varphi - \mu\Delta t/\hbar)}}{\sqrt{N!M!}} \\ &\times \langle N(t) \rangle^{\frac{N+M}{2}} (1-j\Delta t)^{\frac{N+M}{2}}, \end{aligned} \quad (17)$$

which indeed satisfy Eq. (8).

We now discuss the compatibility with the SSR, which might raise the objection that the CSIB would not be realized because superpositions between states with different values of N are forbidden for massive bosons. To show that this intuitive objection is wrong, it is sufficient to give one counter example. Suppose that there is another box, which also contains condensed bosons, in the same room. The total system consists of two boxes and the environment. According to the SSR, the wavefunction of the total system $|\Phi\rangle_{\text{total}}$ should be a superposition of states that have the same number of bosons, $N_{\text{total}} = N + N' + N_E = \text{fixed}$, where N' denotes the number of bosons in the second box. Consider the following state, which satisfies this constriction;

$$\begin{aligned} |\Phi\rangle_{\text{total}} &= \sum_{N, N', \ell} e^{-|\alpha|^2/2 - |\alpha'|^2/2} \alpha^N \alpha'^{N'} C_\ell / \sqrt{N!N'!} \\ &\times |N, G\rangle \otimes |N', G'\rangle \otimes |N_{\text{total}} - N - N', \ell\rangle_E. \end{aligned} \quad (18)$$

Here, $\alpha = |\alpha|e^{i\varphi}$, $\alpha' = |\alpha'|e^{i\varphi'}$, and C_ℓ is a complex number, where ℓ is a quantum number labeling states of the environment $|M, \ell\rangle_E$ which has M bosons. Regarding the phases φ and φ' , only the relative value $\varphi - \varphi' \equiv \theta$ has a physical meaning. We thus take $\varphi' = 0$ henceforth. Equation (18) yields the reduced density operator of the first box as $\hat{\rho} = \sum_N e^{-|\alpha|^2} (|\alpha|^{2N} / N!) |N, G\rangle\langle N, G|$. It is easy to show that this is identical to

$$\hat{\rho} = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} ||\alpha|e^{i\theta}, G\rangle\langle \alpha|e^{i\theta}, G|. \quad (19)$$

Although this $\hat{\rho}$ represents a mixed state of the CSIB, we note that *it does not contain the maximum information* on the state in the box. The lacking information is that the phase relative to the condensate in the second box is φ . Hence, the maximum information is Eq. (19) plus $\theta = \varphi$. This combined information is concisely expressed as $\hat{\rho} = ||\alpha|e^{i\varphi}, G\rangle\langle \alpha|e^{i\varphi}, G|$, which agrees with Eq. (12). Namely, Eq. (12) is better than Eq. (19) because it contains more information. This example demonstrates that Eq. (12) is compatible with the SSR in realistic cases

where the box exchanges bosons with the environment. Only in the limiting case where the box is completely closed, should the SSR be crucial, and the NSIB would be realized if the temperature $T \rightarrow 0$ [14].

We have established that the CSIB is a robust pure state of interacting many bosons. We finally discuss its implications. A stability of macroscopic wavefunctions is often discussed as their “stiffness” [3]. Note, however, that the stiffness is different from the robustness of the present work, because, e.g., in the limit of vanishing boson-boson interactions the stiffness disappears [3] whereas the robustness of the CSIB survives. The robustness is generalization of the robustness of coherent states of $f = 1$ systems [1,2]. It is thus natural to expect for $f \gg 1$ systems that *some* coherent state would be robust. However, it was not known *what* coherent state is robust: there are many choices of the coordinate by which a coherent state is defined. Since Eq. (3) yields

$$(\hat{\Xi}/\xi)|\alpha, G\rangle = \alpha|\alpha, G\rangle, \quad (20)$$

the present work has revealed that the robust coherent state is the one defined by $\hat{\Xi}/\xi$. In this sense, $\hat{\Xi} + \hat{\Xi}^\dagger$ is the “natural coordinate” of interacting many bosons. The condensation of bosons are often characterized by the off-diagonal long-range order (ODLRO) that is defined by $\langle \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}') \rangle = \text{finite for } |\mathbf{r} - \mathbf{r}'| \sim V^{-1/3}$ [3]. Using Eqs. (2)-(5) we can show that the CSIB, NSIB, NPIB, and the Bogoliubov’s ground state all have the ODLRO. Hence, the present work has revealed that the ODLRO does not necessarily imply the robustness. Furthermore, all these states have the same energy, i.e., the differences of $\langle \hat{H} \rangle$ are only $\mathcal{O}(1/V)$ for the same value of $\langle N \rangle$ [15]. For example, let $E_{N,G}$ be the eigenenergy of the NSIB, $\hat{H}|N, G\rangle = E_{N,G}|N, G\rangle$, then we can easily show from Eq. (15), neglecting terms of $\mathcal{O}(1/V)$, that $\langle \alpha, G | \hat{H} | \alpha, G \rangle = E_{|\alpha|^2, G} = E_{\langle N \rangle, G}$. Therefore, the robustness of the CSIB is *not* due to an energy difference, but to natures of wavefunctions. Since interactions with the environment are finite in most physical systems, we argue that only the robust state, CSIB, should be realized as a macroscopic pure state. Since the (relative) phase of the CSIB is almost definite [9], the global gauge symmetry is then broken. Although V is finite, we are thus led to the symmetry breaking (SB) by considering the robustness. This suggests that quantum phase transitions may have more profound origins than singularities that are developed as $V \rightarrow \infty$. A conventional trick to get SB states for boson condensates is to introduce a SB field η , which couples to $\hat{\psi}$ as $\hat{H}_\eta = \int d^3\mathbf{r}(\eta^* \hat{\psi} + \eta \hat{\psi}^\dagger)$. However, η is usually considered as an unphysical field [3,16,17], and it was sometimes argued that SB states were meaningless because they look against the SSR [17]. In contrast, the present work gives a physical reasoning for the SB, assuming only physical interactions, and shows the compatibility with the SSR.

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